

Understanding Ozone Pollution:

A Comparison of Chemical Mechanisms

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Motivation

- ▶ Importance of O_3 production chemistry representation – future emission scenarios.
- ▶ Compare different O_3 chemistry representations used in chemical transport models.
- ▶ Determine effects on O_3 production by comparing treatment of Volatile Organic Compounds (VOCs) degradation products.

Approach

- ▶ Tagged Ozone Production Potentials (TOPPs) [1] calculated over 7 days for VOCs common to urban environments.

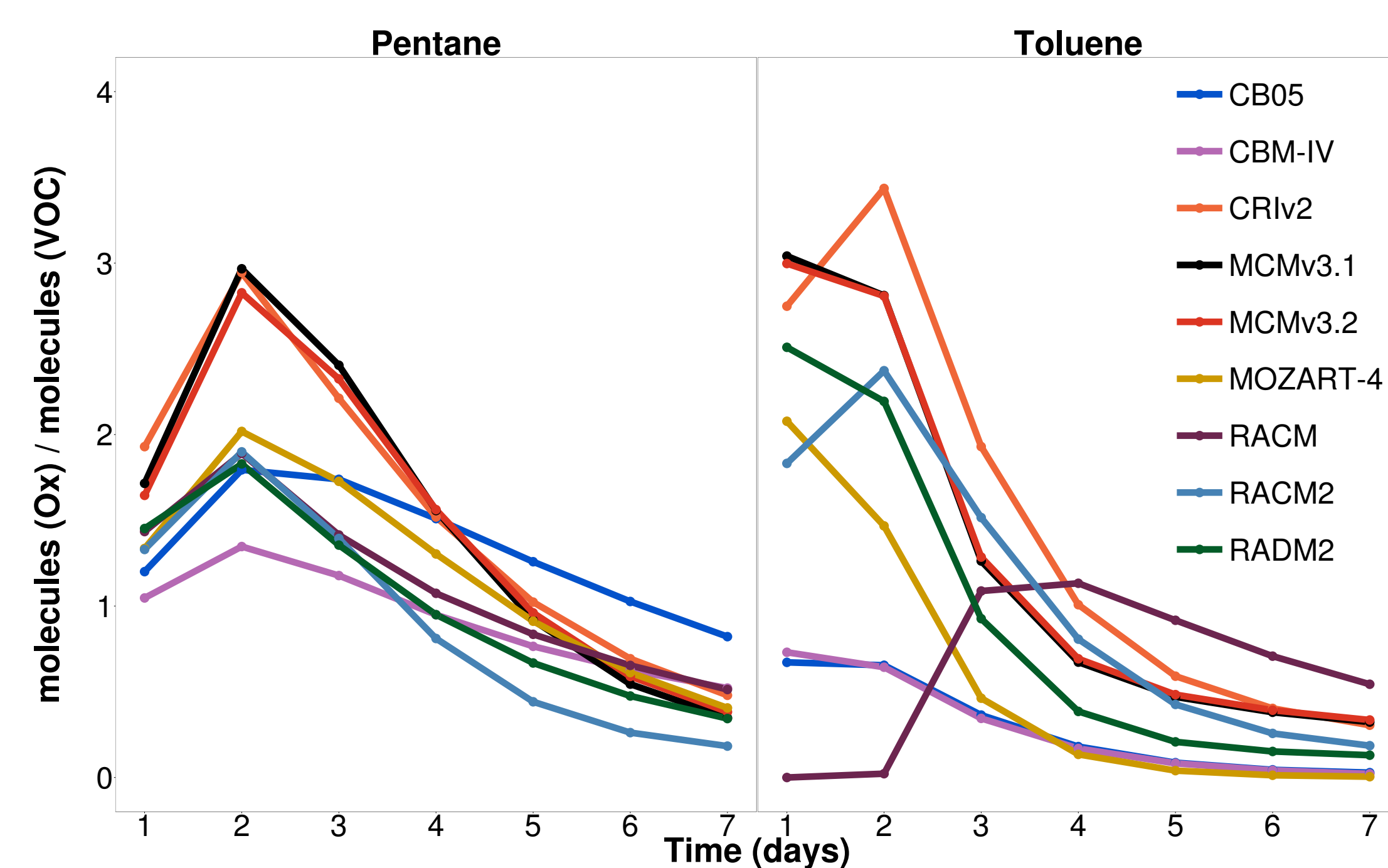
- ▶ Following mechanisms are compared to near-explicit MCM v3.2.

MCM v3.1	CRI v2	CBM-IV	CB05
RADM2	RACM	RACM2	MOZART-4

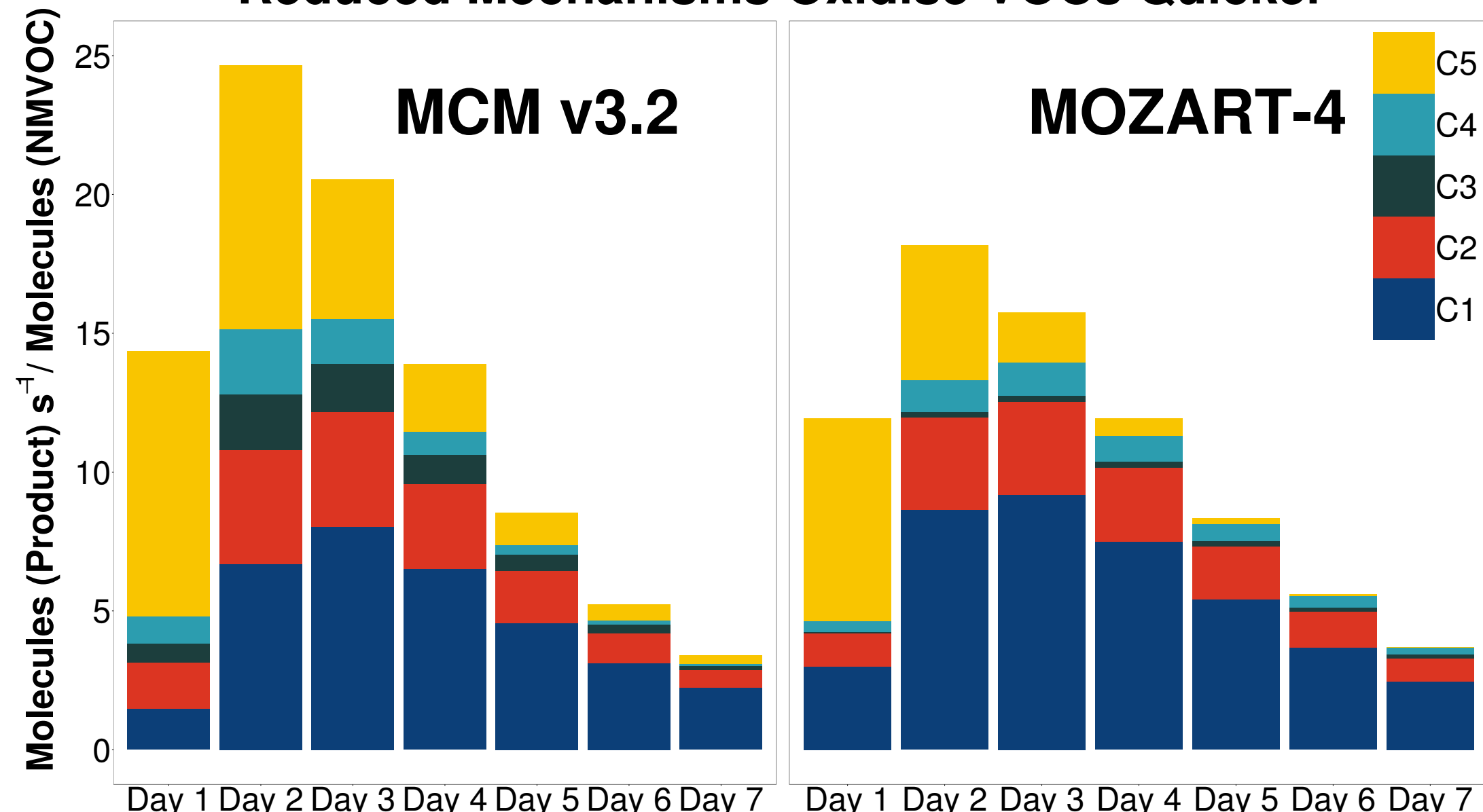
- ▶ O_x ($= O_3 + NO_2$) production allocated to emitted VOC by 'tagging' its organic degradation products.

Results

TOPP Time Series: Large Spread between Mechanisms

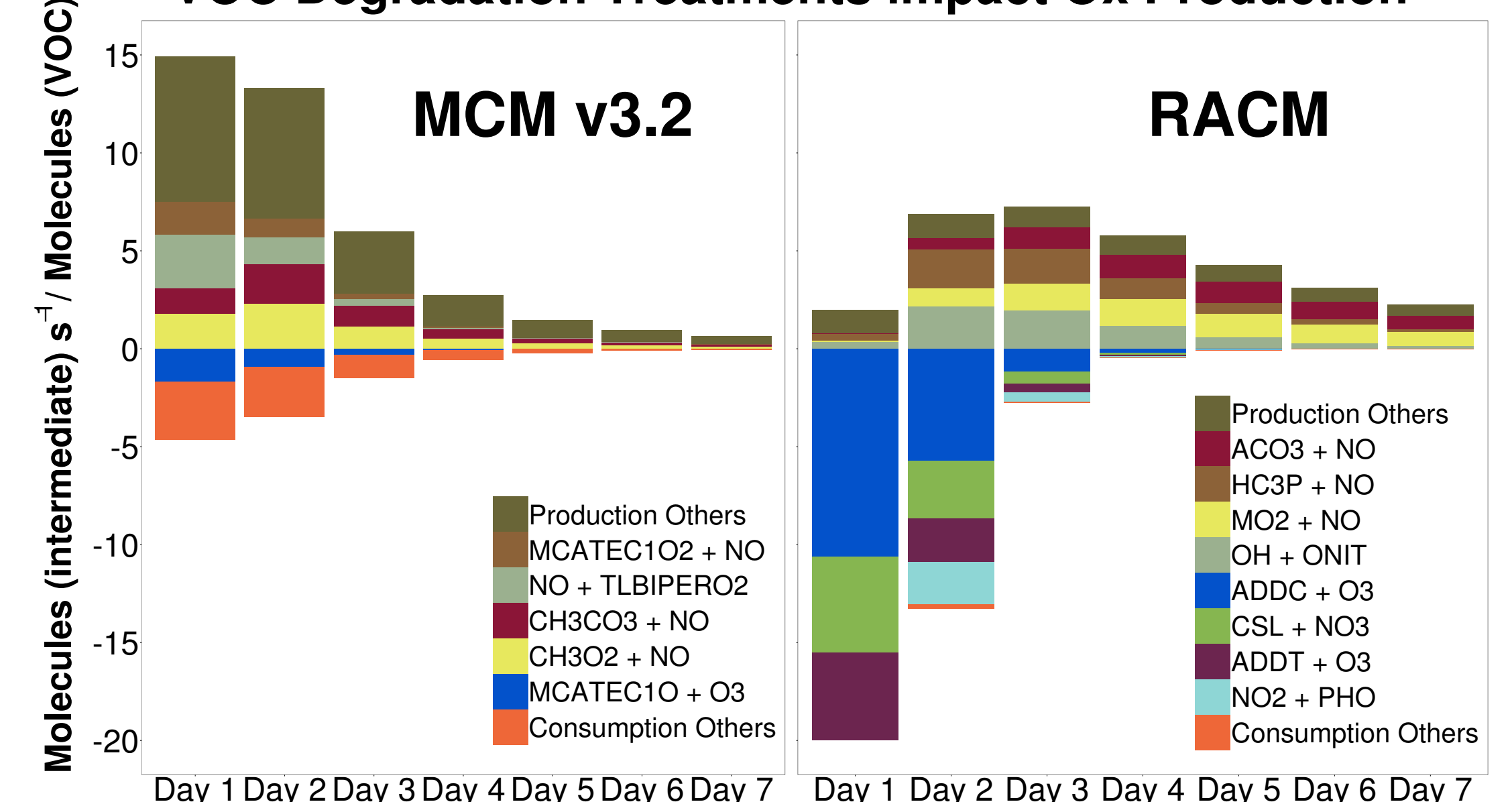


Pentane Ox Production by Carbon Number: Reduced Mechanisms Oxidise VOCs Quicker



Toluene Organic Ox Budgets:

VOC Degradation Treatments impact Ox Production



Conclusions

- ▶ More explicit mechanisms produce more O_x than less explicit mechanisms.
- ▶ VOCs broken down into smaller fragments quicker in less-explicit mechanisms resulting in less O_x production.
- ▶ First day O_x production from VOCs similar between many mechanisms, larger differences over time.
- ▶ Differences in VOC degradation treatments impacts on O_x production – RACM aromatic chemistry.

References

- [1] T. M. Butler, M. G. Lawrence, D. Taraborrelli, and J. Lelieveld. Multi-day ozone production potential of volatile organic compounds calculated with a tagging approach. Atmospheric Environment, 45(24):4082–4090, 2011.



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